INL/CON-06-11777
PREPRINT

Fluid Flow, Solute Mixing and Precipitation in Porous Media

INRA 2006 Environmental Subsurface Science Symposium

G.D. Redden
Y. Fang
T.D. Scheibe
A.M. Tartakovsky
D.T. Fox
Yoshiko Fujita
T.A. White

September 2006

The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance

FLUID FLOW, SOLUTE MIXING AND PRECIPITATION IN POROUS MEDIA

G.D. Redden[1], Y. Fang[2], T.D. Scheibe[2], A.M. Tartakovsky[2], D.T. Fox[1], Yoshiko Fujita[1] and T.A. White[1]

[1]Idaho National Laboratory, Idaho Falls, ID, USA

[2]Pacific Northwest National Laboratory, Richland, WA, USA

Reactions that lead to the formation of mineral precipitates, colloids or growth of biofilms in porous media often depend on the molecular-level diffusive mixing. For example, for the formation of mineral phases, exceeding the saturation index for a mineral is a minimum requirement for precipitation to proceed. Solute mixing frequently occurs at the interface between two solutions each containing one or more soluble reactants, particularly in engineered systems where contaminant degradation or modification or fluid flow are objectives. Although many of the fundamental component processes involved in the deposition or solubilization of solid phases are reasonably well understood, including precipitation equilibrium and kinetics, fluid flow and solute transport, the deposition of chemical precipitates, biofilms and colloidal particles are all coupled to flow, and the science of such coupled processes is not well developed. How such precipitates (and conversely, dissolution of solids) are distributed in the subsurface along flow paths with chemical gradients is a complex and challenging problem. This is especially true in systems that undergo rapid change where equilibrium conditions cannot be assumed, particularly in subsurface systems where reactants are introduced rapidly, compared to most natural flow conditions, and where mixing fronts are generated. Although the concept of dispersion in porous media is frequently used to approximate mixing at macroscopic scales, dispersion does not necessarily describe pore-level or molecular level mixing that must occur for chemical and biological reactions to be possible.

An example of coupling between flow, mixing and mineral precipitation, with practical applications to controlling fluid flow or contaminant remediation in subsurface environments is shown in the mixing zone between parallel flowing solutions. Two- and three-dimensional experiments in packed-sand media were conducted where solutions containing calcium and carbonate ions came into contact along a parallel flow boundary and mixed by dispersion and diffusion. The result is the propagation of calcium carbonate precipitates along the solution-solution boundary in the direction of flow. As carbonate precipitates fill the pore space mixing of the two solutions is restricted and therefore precipitation, flow, and transport are coupled. The distribution of carbonate phases is a complex interaction involving precipitation and dissolution kinetics, which are functions of pore-scale saturation indices and solute ratios, heterogeneous vs. homogeneous nucleation and growth mechanisms and changes in porosity and flow. Experimental and modeling results illustrate challenges in understanding the macroscopic and microscopic phenomena that depend on solute mixing, the relevance of molecular and pore-scale processes to the macroscopic behavior, and potential impact on metal mobility in porous media. Mineral precipitation and changes in porosity are simulated at the pore-scale using the Smooth Particle Hydrodynamics method. Macroscopic simulations were performed using discretized, continuum-scale modeling with parameterization representing macroscopic media properties. One of the modeling goals is to use pore-scale simulations to provide the basis for parameterization of macroscopic (more practical) model predictions.

Relevant topic areas:
Subsurface Contamination, Simulations/Modeling, Impact of biogeochemistry on flow and transport, Subsurface fate & transport of organic pollutants, heavy metals, and radionuclides,

Geochemistry, Environmental Contaminants, **Experiments to understand coupled processes in the subsurface**, Approaches to containment stabilization, Development of improved remediation technologies